

STABILITY OF A FORCE-BASED HYBRID METHOD IN THREE DIMENSION WITH SHARP INTERFACE

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ABSTRACT. We study a force-based hybrid method that couples atomistic model with Cauchy-Born elasticity model with sharp transition interface. We identify stability conditions that guarantee the convergence of the hybrid scheme to the solution of the atomistic model with second order accuracy, as the ratio between lattice parameter and the characteristic length scale of the deformation tends to zero. Convergence is established for the three dimensional system without defects, with general finite range atomistic potential and simple lattice structure. The key ingredient of the proof is regularity and stability analysis of elliptic finite difference schemes. We apply the result to an atomistic-to-continuum scheme for a triangular lattice with harmonic interactions.

1. INTRODUCTION

Multiscale methods couple together atomistic and continuum models have received intense investigations in recent years (see e.g. [1, 10, 21, 29, 30]). Generally speaking, there are two main categories of methods coupling atomistic and continuum models: energy-based and force-based methods. The energy-based methods employ an energy that is a mixture of atomistic energy and continuum elastic energy. The energy functional is then minimized subject to suitable boundary conditions to obtain the deformed state of the system. The force-based methods work instead at the level of force balance equations. The forces derived from atomistic and continuum models are coupled together. The force balance equations supplemented with suitable boundary conditions are solved to obtain the deformed state of the system.

From a numerical analysis point of view, the key issue for these multiscale methods is the consistency and stability analysis of the coupled schemes [10, Chapter 7]. In this paper, we study force-based atomistic-to-continuum hybrid methods in two and three dimension with sharp transition between the atomistic and continuum regions. In our previous work [20], we developed the stability analysis in general

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dimension for a force-based atomistic-to-continuum method with smooth transition between the two regions. The main focus of the current paper is to extend the stability analysis of [20] to hybrid schemes with sharp interface between atomistic and continuum models.

Comprehensive reviews for force-based hybrid methods can be found in [23, Section 5 and Section 6] and [29, Section 12.5]. A class of force-based methods uses a handshake region (transition region) between the atomistic and continuum regions. A representative of such methods is the concurrent AtC coupling method (AtC) developed in a series of papers [3, 4, 13, 25], blending the continuum stress and the atomistic forces. The method recently proposed and analyzed by the authors in [20] shares certain common traits with the AtC method. It is proved to be stable and convergent with optimal convergence rate. The numerical implementation of the method can be found in [33].

As a representative for force-based methods without handshake region, the FEAt method of Kohlhoff, Gumbsch and Fischmeister [17] is perhaps one of the earliest force-based methods. In this method, an elasticity model is coupled with an atomistic model. The FEAt method does not use a handshake region: the transition between the atomistic model and the continuum model is sharp. This kind of coupling is generalized in CADD method [27], which uses the discrete dislocation model in the continuum region.

One of the main advantages of the force-based methods is that consistency is achieved with fairly simple construction. Hence the main focus of analysis of such methods is stability. The stability for one-dimensional force-based method was analyzed in [8, 9]. The generalization to higher dimension is quite nontrivial due to the complications of lattice structures and atomistic interaction potentials. The main idea in our previous paper [20] and the current paper is to establish linearized H^2 -stability of the hybrid scheme by viewing the scheme as a nonlinear elliptic finite difference system and applying the elliptic regularity estimates for such system. The recent work [19] by Li, Luskin and Ortner proved linearized H^1 -stability for methods with smooth coupling under certain stability conditions. These conditions however were not yet known how to check explicitly [19]. They also studied how the size of the transition region affects the stability.

For atomistic-to-continuum hybrid method with sharp interface studied in this paper, stability might fail at the interface. Therefore, to make sure that the hybrid scheme is convergent, we need to check the stability conditions at the interface for the coupling schemes. We shall identify the interface stability conditions as analogs of the complementing boundary conditions in elliptic PDE literature. From a physical perspective, these stability conditions amount to check whether there exists nontrivial surface phonon at the interface of the two schemes. To some

extent, these stability conditions are analogous to the famous Gustafsson-Kreiss-Sundström stability conditions [14] for finite difference approximations of mixed initial/boundary value problems.

The main result in this paper is the linearized H^2 -stability and convergence of atomistic-to-continuum hybrid method under the stability conditions. The essential ingredients are regularity and stability analysis of finite difference schemes. As a consequence of our main results, we will show that a force-based atomistic-to-continuum coupling for a 2D triangular lattice with next-nearest neighbor harmonic interaction is stable and hence convergent, when the interface between the atomistic and continuum regions is parallel to the $(1, \sqrt{3})/2$ direction of the lattice. Let us finally remark that while we focus on hybrid schemes coupling atomistic and nonlinear elasticity models, the ideas and techniques in the current paper can be extended to other force-based hybrid methods, e.g., the force-based coupling of peridynamics and nonlinear elasticity proposed in [26].

Before we formulate the problem and state our main result, we introduce some preliminaries and notations.

1.1. Lattice function and norms. We will consider only Bravais lattices in this work, which is denoted as \mathbb{L} . Let $\{a_j\}_{j=1}^d \subset \mathbb{R}^d$ be the basis vectors of \mathbb{L} , and d be the dimension,

$$\mathbb{L} = \left\{ x \in \mathbb{R}^d \mid x = \sum_j n_j a_j, n \in \mathbb{Z}^d \right\}.$$

Let $\{b_j\}_{j=1}^d \subset \mathbb{R}^d$ be the reciprocal basis vectors satisfying $a_j \cdot b_k = 2\pi\delta_{jk}$, where δ_{jk} is the standard Kronecker delta symbol. The reciprocal lattice \mathbb{L}^* is then

$$\mathbb{L}^* = \left\{ x \in \mathbb{R}^d \mid x = \sum_j n_j b_j, n \in \mathbb{Z}^d \right\}.$$

We take a computational domain

$$\Omega = \left\{ \sum_{j=1}^d x_j a_j \mid x \in [0, 1]^d \right\},$$

and let Ω_ε be a grid mesh in Ω with mesh size $\varepsilon = 1/(2N)$, $N \in \mathbb{Z}_+$:

$$\Omega_\varepsilon = \left\{ x_\nu = \varepsilon \sum_{j=1}^d \nu_j a_j \mid \nu \in \mathbb{Z}^d, 0 \leq \nu_j < 2N \right\}.$$

Using the reciprocal basis $\{b_j\}$, we define

$$\mathbb{L}_\varepsilon^* = \left\{ \xi = \sum_{j=1}^d k_j b_j \mid k \in \mathbb{Z}^d, -N \leq k_j < N \right\}.$$

We will identify functions defined on Ω_ε with their periodic extensions in this work, *i.e.*, we consider the periodic boundary condition. General boundary conditions will be left for future work.

For $\mu \in \mathbb{Z}^d$, we define the translation operator T_ε^μ as

$$(T_\varepsilon^\mu u)(x) = u(x + \varepsilon \mu_j a_j) \quad \text{for } x \in \mathbb{R}^d,$$

where the index summation convention is used. We define the forward and backward difference operators as

$$D_{\varepsilon, \mu}^+ = \varepsilon^{-1}(T_\varepsilon^\mu - I) \quad \text{and} \quad D_{\varepsilon, \mu}^- = \varepsilon^{-1}(I - T_\varepsilon^{-\mu}),$$

where I denotes the identity operator. We say α is a multi-index, if $\alpha \in \mathbb{Z}^d$ and $\alpha \geq 0$. We will use the notation $|\alpha| = \sum_{j=1}^d \alpha_j$. For a multi-index α , the difference operator D_ε^α is given by

$$D_\varepsilon^\alpha = \prod_{j=1}^d (D_{\varepsilon, e_j}^+)^{\alpha_j},$$

where $\{e_j\}_{j=1}^d$ are the canonical basis of \mathbb{R}^d (columns of a $d \times d$ identity matrix).

We will use various norms for functions defined on Ω_ε . For integer $k \geq 0$, define the difference norm

$$\|u\|_{\varepsilon, k}^2 = \sum_{0 \leq |\alpha| \leq k} \varepsilon^d \sum_{x \in \Omega_\varepsilon} |(D_\varepsilon^\alpha u)(x)|^2.$$

It is clear that $\|\cdot\|_{\varepsilon, k}$ is a discrete analog of Sobolev norm associated with $H^k(\Omega)$. Hence, we denote the corresponding spaces of lattice functions as $H_\varepsilon^k(\Omega)$ and $L_\varepsilon^2(\Omega)$ when $k = 0$. We also need the uniform norms on Ω_ε , which is given by

$$\begin{aligned} \|u\|_{L_\varepsilon^\infty} &= \max_{x \in \Omega_\varepsilon} |u(x)|, \\ \|u\|_{W_\varepsilon^{k, \infty}} &= \sum_{0 \leq |\alpha| \leq k} \max_{x \in \Omega_\varepsilon} |(D_\varepsilon^\alpha u)(x)|. \end{aligned}$$

Recall that we identify lattice function u with its periodic extension to function defined on $\varepsilon\mathbb{L}$, and hence differences of the lattice functions are well-defined. These norms may be extended to vector-valued functions as usual. For $k > d/2$, we have the discrete Sobolev inequality $\|u\|_{L_\varepsilon^\infty} \lesssim \|u\|_{\varepsilon, k}$. Here and throughout this paper, we denote $A \lesssim B$ if $A \leq CB$ with C an absolute constant.

The discrete Fourier transform for a lattice function u is given for $\xi \in \mathbb{L}_\varepsilon^*$ by

$$(1.1) \quad \widehat{u}(\xi) = \left(\frac{\varepsilon}{2\pi}\right)^d \sum_{x \in \Omega_\varepsilon} e^{-i\xi \cdot x} u(x).$$

By the Fourier inversion formula, for $x \in \Omega_\varepsilon$,

$$(1.2) \quad u(x) = \sum_{\xi \in \mathbb{L}_\varepsilon^*} e^{ix \cdot \xi} \widehat{u}(\xi).$$

We will use a symbol introduced by Nirenberg in [24], which plays the same role for the difference operators as $\Lambda^2(\xi) = 1 + \Lambda_0^2(\xi) = 1 + |\xi|^2$ for the differential operators. For $\varepsilon > 0$, let

$$\Lambda_{j, \varepsilon}(\xi) = \frac{1}{\varepsilon} |e^{i\varepsilon \xi_j} - 1|, \quad j = 1, \dots, d,$$

and

$$\Lambda_\varepsilon^2(\xi) = 1 + \Lambda_{0,\varepsilon}^2(\xi) = 1 + \sum_{j=1}^d \Lambda_{j,\varepsilon}^2(\xi) = 1 + \sum_{j=1}^d \frac{4}{\varepsilon^2} \sin^2\left(\frac{\varepsilon \xi_j}{2}\right).$$

It is not hard to check for any $\xi \in \mathbb{L}_\varepsilon^*$, there holds

$$(1.3) \quad c\Lambda^2(\xi) \leq \Lambda_\varepsilon^2(\xi) \leq \Lambda^2(\xi),$$

where the positive constant c depends on $\{b_j\}$.

1.2. Atomistic model and Cauchy-Born rule. We consider classical empirical potentials: For atoms located at $\{y_1, \dots, y_K\}$, the interaction potential energy between the atoms is given by $V(y_1, \dots, y_K)$, where V often takes the form

$$V(y_1, \dots, y_K) = \sum_{i,j} V_2(y_i/\varepsilon, y_j/\varepsilon) + \sum_{i,j,k} V_3(y_i/\varepsilon, y_j/\varepsilon, y_k/\varepsilon) + \dots,$$

where we have omitted interactions of more than three atoms.

As in our previous work [20], we will make the following assumptions on the potential function V :

- (1) V is translation invariant.
- (2) V is invariant with respect to rigid body motion.
- (3) V is smooth in a neighborhood of the equilibrium state.
- (4) V has finite range and consequently we will consider only interactions that involve a finite number of atoms.

For simplicity of notation and clarity of presentation, our presentation will be limited to potentials that contain only two-body and three-body potentials, and we will only make explicit the three-body terms in the expressions for the potential. It is straightforward to extend our results to potentials with interactions of more atoms that satisfy the above assumptions by following the discussion on the three-body terms. As the potential function V is a function of atom distances and angles by invariance with respect to rigid body motion, we may write

$$V_3(y_i, y_j, y_k) = V_3\left(|y_i - y_j|^2, |y_i - y_k|^2, \langle y_i - y_j, y_i - y_k \rangle\right),$$

where $\langle \cdot, \cdot \rangle$ denotes the inner product over \mathbb{R}^d .

We assume that the atoms located at Ω_ε are in equilibrium, with $x \in \Omega_\varepsilon$ the equilibrium position. Positions of the atoms under deformation will be viewed as a function defined over Ω_ε , which is denoted as $y(x) = x + u(x)$. Hence, $u : \Omega_\varepsilon \rightarrow \mathbb{R}^d$ is the displacement of the atoms. Define the space of the displacement field as

$$X_\varepsilon = \left\{ u : \Omega_\varepsilon \rightarrow \mathbb{R}^d \mid \sum_{x \in \Omega_\varepsilon} u(x) = 0 \right\}.$$

The atomistic problem is formulated as follows. Given force field $f_\varepsilon : \Omega_\varepsilon \rightarrow \mathbb{R}^d$, find $u \in X_\varepsilon$ such that

$$(1.4) \quad u = \arg \min_{u \in X_\varepsilon} I_{\text{at}}(u),$$

where

$$I_{\text{at}}(u) = \frac{1}{3!} \varepsilon^d \sum_{x \in \Omega_\varepsilon} \sum_{(s_1, s_2) \in S} V_{(s_1, s_2)}[x + u] - \varepsilon^d \sum_{x \in \Omega_\varepsilon} f_\varepsilon(x) u(x),$$

and

$$V_{(s_1, s_2)}[y] = V \left(|D_{s_1}^+ y(x)|^2, |D_{s_2}^+ y(x)|^2, \langle D_{s_1}^+ y(x), D_{s_2}^+ y(x) \rangle \right).$$

Here S is the set of all possible (s_1, s_2) within the range of the potential. By our assumptions, S is a finite set. We only make explicit the three-body terms in the potential as mentioned before. In I_{at} , ε^d is a normalization factor, so that I_{at} is actually the energy of the system per atom.

The Euler-Lagrange equation for the atomistic problem is

$$(1.5) \quad \mathcal{F}_{\text{at}}[u](x) = f_\varepsilon(x) \quad x \in \Omega_\varepsilon,$$

where

$$\begin{aligned} \mathcal{F}_{\text{at}}[u](x) = & \sum_{(s_1, s_2) \in S} \left(D_{s_1}^- (2\partial_1 V_{(s_1, s_2)}[y](x) D_{s_1}^+ y(x) + \partial_3 V_{(s_1, s_2)}[y](x) D_{s_2}^+ y(x)) \right. \\ & \left. + D_{s_2}^- (2\partial_2 V_{(s_1, s_2)}[y](x) D_{s_2}^+ y(x) + \partial_3 V_{(s_1, s_2)}[y](x) D_{s_1}^+ y(x)) \right), \end{aligned}$$

where for $i = 1, 2, 3$, we denote

$$\partial_i V_{(s_1, s_2)}[y](x) = \partial_i V \left(|D_{s_1}^+ y(x)|^2, |D_{s_2}^+ y(x)|^2, \langle D_{s_1}^+ y(x), D_{s_2}^+ y(x) \rangle \right)$$

the partial derivative with respect to the i -th argument of V .

To guarantee the solvability of (1.5), we assume that f_ε takes the following form:

$$f_\varepsilon(x) \equiv \varepsilon^{-d} \int_{x+\varepsilon\Gamma} f(z) \, dz, \quad x \in \Omega_\varepsilon,$$

where $f(x)$ is a function defined on Ω with zero mean. This makes sure that $f_\varepsilon(x)$ satisfies

$$\sum_{x \in \Omega_\varepsilon} f_\varepsilon(x) = \varepsilon^{-d} \int_{\Omega} f(x) \, dx = 0.$$

To introduce the Cauchy-Born elasticity problem [5, 11, 12], we fix more notations. For any positive integer k , we denote by $W^{k,p}(\Omega; \mathbb{R}^d)$ the Sobolev space of mappings $u: \Omega \rightarrow \mathbb{R}^d$ such that $\|u\|_{W^{k,p}}$ is finite, and by $W_{\#}^{k,p}(\Omega; \mathbb{R}^d)$ the Sobolev space of periodic functions whose distributional derivatives of order less than k are in $L^p(\Omega)$. For any $p > d$ and $m \geq 0$, we define X as

$$X = \left\{ u : \Omega \rightarrow \mathbb{R}^d \mid u \in W^{m+2,p}(\Omega; \mathbb{R}^d) \cap W_{\#}^{1,p}(\Omega; \mathbb{R}^d), \int_{\Omega} u = 0 \right\}.$$

The Cauchy-Born elasticity problem is formulated as follows. Find $u \in X$ such that

$$(1.6) \quad u = \arg \min_{u \in X} I(u),$$

where the total energy functional I is given by

$$I(u) = \int_{\Omega} (W_{\text{CB}}(\nabla u(x)) - f(x)u(x)) \, dx.$$

Here the Cauchy-Born stored energy density W_{CB} is given by

$$W_{\text{CB}}(A) = \frac{1}{3!} \sum_{(s_1, s_2) \in S} W_{(s_1, s_2)}(A),$$

where for $A \in \mathbb{R}^{d \times d}$,

$$W_{(s_1, s_2)}(A) = V \left(|s_1 + s_1 A|^2, |s_2 + s_2 A|^2, \langle s_1 + s_1 A, s_2 + s_2 A \rangle \right).$$

The range S is the same as that in the atomistic potential function.

The Euler-Lagrange equation for the Cauchy-Born elasticity model is

$$(1.7) \quad \mathcal{F}_{\text{CB}}[u](x) = f(x),$$

where

$$\mathcal{F}_{\text{CB}}[u](x) = -\operatorname{div} \left(D_A W_{\text{CB}}(\nabla u(x)) \right).$$

Here $D_A W_{\text{CB}}(A)$ denotes the derivative of $W_{\text{CB}}(A)$ with respect to A .

Since we are primarily interested in the coupling between the atomistic and continuum models, we will take the finite element mesh \mathcal{T}_ε as a triangulation of Ω_ε with each atom site as an element vertex. The triangulation is translational invariant. The approximation space \tilde{X}_ε is defined as

$$\tilde{X}_\varepsilon = \left\{ u \in W_{\#}^{1,p}(\Omega; \mathbb{R}^d) \mid u|_T \in P_1(T), \forall T \in \mathcal{T}_\varepsilon \right\},$$

where $P_1(T)$ is the space of linear functions on the element T . We denote by \mathcal{F}_ε the force from finite element approximation of Cauchy-Born elasticity problem (1.6).

1.3. Formulation of force-based hybrid method with sharp interface. We are ready to formulate the force-based hybrid method. We take a continuum region

$$\Omega_c = \left\{ \sum_{j=1}^d x_j a_j \mid 0 \leq x_1 < 1/2, 0 \leq x_j < 1, j = 2, \dots, d \right\},$$

and denote ϱ the characteristic function associated with Ω_c : $\varrho(x) = 1$ if $x \in \Omega_c$. $\Omega_a = \Omega \setminus \Omega_c = \{x \mid \varrho(x) = 0\}$ is the atomistic region. Note that the continuum and atomistic regions are separated by two hyperplanes $\{x_1 = 0\}$ and $\{x_1 = 1/2\}$ as a result of periodic boundary condition. The simple geometry here is chosen for simplicity of presentation, using localization techniques as in [18] (see also the proof of Theorem 3 below), the analysis can be generalized to any Ω_c with smooth boundary.

We consider a force field defined as

$$(1.8) \quad \mathcal{F}_{\text{hy}}[u](x) \equiv (1 - \varrho(x))\mathcal{F}_{\text{at}}[u](x) + \varrho(x)\mathcal{F}_{\varepsilon}[u](x), \quad x \in \Omega_{\varepsilon}.$$

Due to the choice of ϱ , in the atomistic region Ω_a , the force acting on the atom is just that of atomistic model, while in the continuum region Ω_c , the force is calculated from finite element approximation of the Cauchy-Born elasticity. Since ϱ is taken to be the characteristic function, we consider here a hybrid method with sharp interface, i.e., there is no transition or buffer region between the atomistic and continuum regions.

Given a loading f_{ε} , we find $u \in X_{\varepsilon}$ such that

$$(1.9) \quad (\Pi_{\varepsilon}\mathcal{F}_{\text{hy}}[u])(x) = f_{\varepsilon}(x) \quad x \in \Omega_{\varepsilon},$$

where for a lattice function g , Π_{ε} projects g to a function with zero mean:

$$(\Pi_{\varepsilon}g)(x) := g(x) - \varepsilon^d \sum_{x' \in \Omega_{\varepsilon}} g(x').$$

As in [20], the convergence of the hybrid scheme is tightly connected with the linear stability of the finite difference scheme. Thus, we will study the linearized operator of \mathcal{F}_{hy} . Let us denote $\mathcal{H}_{\text{hy}}[u]$ the linearization of \mathcal{F}_{hy} at state u : $\mathcal{H}_{\text{hy}}[u] = \frac{\delta \mathcal{F}_{\text{hy}}}{\delta u}$, so that $\mathcal{H}_{\text{hy}}[u]$ is a linear operator acting on a lattice functions w , which is given by

$$\mathcal{H}_{\text{hy}}[u]w = \lim_{t \rightarrow 0} \frac{\partial \mathcal{F}_{\text{hy}}}{\partial t}[u + tw].$$

We will rewrite the operator \mathcal{H}_{hy} in the form of a difference operator as

$$\mathcal{H}_{\text{hy}}[u] = \sum_{\mu \in \mathcal{A}} h_{\text{hy}}[u](x, \mu) T^{\mu},$$

where the coefficient $h_{\text{hy}}[u](x, \mu)$ is a d by d matrix (probably asymmetric) for each x and $\mu \in \mathcal{A}$, which is given by

$$(1.10) \quad (h_{\text{hy}}[u])_{\alpha\beta}(x, \mu) = \frac{\partial (\mathcal{F}_{\text{hy}}[u])_{\alpha}(x)}{\partial (T^{\mu}u)_{\beta}(x)},$$

where $\alpha, \beta = 1, \dots, d$ are indices. Here \mathcal{A} is the stencil of the difference operator, which is finite by assumptions on the atomistic potential. By the definition of \mathcal{F}_{hy} , we have

$$(1.11) \quad h_{\text{hy}}[u](x, \mu) = (1 - \varrho(x))h_{\text{at}}[u](x, \mu) + \varrho(x)h_{\varepsilon}[u](x, \mu),$$

where $h_{\text{at}}[u]$ and $h_{\varepsilon}[u]$ are given by similar equations as (1.10) with \mathcal{F}_{hy} replaced by \mathcal{F}_{at} and $\mathcal{F}_{\varepsilon}$, respectively.

Define $h_{\text{hy}}[u](x, \xi)$ as the symbol of the pseudo-difference operator $\mathcal{H}_{\text{hy}}[u]$, which is given by

$$h_{\text{hy}}[u](x, \xi) = \sum_{\mu \in \mathcal{A}} h_{\text{hy}}[u](x, \mu) \exp\left(i\varepsilon \sum_j \mu_j a_j \cdot \xi\right) \quad \text{for } \xi \in \mathbb{L}_{\varepsilon}^*,$$

and similarly for $h_\varepsilon[u]$ and $h_{\text{at}}[u]$. By definition, we have for any $x \in \Omega_\varepsilon$,

$$(\mathcal{H}_{\text{hy}}[u]e_k e^{ix \cdot \xi})_j(x) = (h_{\text{hy}}[u])_{jk}(x, \xi) e^{ix \cdot \xi},$$

for $j, k = 1, \dots, d$ and similarly for $h_\varepsilon[u]$ and $h_{\text{at}}[u]$. It is also clear that (1.11) implies

$$(1.12) \quad h_{\text{hy}}[u](x, \xi) = (1 - \varrho(x))h_{\text{at}}[u](x, \xi) + \varrho(x)h_\varepsilon[u](x, \xi).$$

When we linearize \mathcal{F}_{hy} around the equilibrium state $u = 0$, we will simplify the notation as $\mathcal{H}_{\text{hy}} = \mathcal{H}_{\text{hy}}[0]$, $h_{\text{hy}} = h_{\text{hy}}[0]$, and similarly for those defined for atomistic model and finite element discretization of the Cauchy-Born elasticity. By the translation invariance of the total energy I_{at} at the state $u = 0$, we observe that the coefficients of the symbols $h_{\text{at}}(x, \mu)$ and $h_\varepsilon(x, \mu)$ are independent of the position x , i.e.,

$$h_{\text{at}}(x, \mu) = h_{\text{at}}(\mu), \quad h_\varepsilon(x, \mu) = h_\varepsilon(\mu).$$

We also denote \mathcal{H}_{CB} as the linearization of \mathcal{F}_{CB} at the equilibrium state $u = 0$, and define $h_{\text{CB}}(x, \xi)$ as its symbol. Due to the periodic boundary condition, the argument ξ in the symbol $h_{\text{CB}}(x, \xi)$ only takes value in \mathbb{L}^* . Again, due to the translation invariance of the total energy, the symbol h_{CB} is also independent of x .

An elementary calculation shows that the matrices $h_{\text{at}}(\xi)$, $h_\varepsilon(\xi)$ and hence $h_{\text{hy}}(x, \xi)$ are Hermitian for any $\varepsilon > 0$. As in [20], we make the following stability assumption about the atomistic potential:

Assumption A. The matrix $h_{\text{at}}(\xi)$ is positive definite and there exists a positive constant a_{at} such that for any $\varepsilon > 0$ and any $\xi \in \mathbb{L}_\varepsilon^*$,

$$\det h_{\text{at}}(\xi) \geq a_{\text{at}} \Lambda_{0, \varepsilon}^{2d}(\xi).$$

We also recall from [20, Lemma 3.3] that, as a consequence of Assumption A, for sufficiently small ε , the finite element approximation is also linearly stable.

Lemma 1.1. *There exist constants $a, \varepsilon_0 > 0$ that for any $\varepsilon \in (0, \varepsilon_0)$, the symbol $h_\varepsilon(\xi)$ is positive definite and for any $\xi \in \mathbb{L}_\varepsilon^*$,*

$$\det h_\varepsilon(\xi) \geq a \Lambda_{0, \varepsilon}^{2d}(\xi).$$

1.4. Main result. The main focus of the current paper is to establish convergence for the hybrid method with sharp interface as $\varepsilon \rightarrow 0$. In [20], convergence was proved for any short-range interaction potentials when ϱ is a smooth function, or in other words, when the transition region between atomistic and continuum regions is of $\mathcal{O}(\varepsilon^{-1})$. In this paper, as the transition is sharp, we require additional stability conditions to guarantee convergence. Our main result is

Theorem 1 (Convergence). *Under Assumptions A, B, and C, there exist positive constants δ and M , so that for any $p > d$ and $f \in W^{15,p}(\Omega) \cap W_{\#}^{1,p}(\Omega)$ with $\|f\|_{W^{15,p}} \leq \delta$, we have*

$$(1.13) \quad \|y_{\text{hy}} - y_{\text{at}}\|_{\varepsilon,2} \leq M\varepsilon^2.$$

Remark. The Assumption A is a natural stability condition for the atomistic lattice system. Compared with the convergence result in [20], the additional assumptions B and C come from the coupling between the atomistic potential and the finite element discretization at the interface. The two assumptions will be given in Section 3.

Remark. While we do not attempt in this work to optimize the regularity assumption on f , we note that it is easy to relax the assumption to $f \in W^{5,p}(\Omega)$ with $p > d$.

The proof of Theorem 1 follows a similar strategy as in [20]. Actually, once we obtain the stability estimate Theorem 4, the proof of Theorem 1 is essentially the same as that of [20, Theorem 1.1]. The consistency analysis of the scheme follows from that of [20, Section 2] with some immediate adaptations. Observe in particular that the proof of consistency does not depend on the smoothness of ϱ . Hence, we will focus on the linear stability analysis, and omit the consistency part.

The remaining of the paper is organized as follows. In Section 2, we recall the concept of pseudo-difference operators, which will be used to establish the regularity estimates in Section 3. The stability estimate then follows from the regularity estimate combined with consistency, which is presented in Section 4. In Section 5, we apply the general theory to an example of force-based atomistic-to-continuum hybrid method for 2D triangular lattice with next-nearest neighbor harmonic interaction. We make some conclusive remarks in Section 6.

2. REGULARITY OF FINITE DIFFERENCE SCHEME UP TO THE BOUNDARY

To analyze the general hybrid scheme, we will take the viewpoint of our previous work [20] and regard the scheme as a nonlinear finite difference scheme. One of the main ingredients we will use in this paper is the regularity estimates up to the boundary for elliptic difference systems established in [28]. We also note that the regularity estimates of elliptic difference equations and systems have been investigated by several works [6, 15, 16, 18, 22, 28, 31]. For reader's convenience, we recall here the setup and results with some adaptation to the current work.

2.1. Difference operators. We write a difference operator L_ε in the form of

$$(2.1) \quad (L_\varepsilon u)(x) = \sum_{\mu \in \mathcal{A}} l_\varepsilon(x, \mu) (T_\varepsilon^\mu u)(x),$$

where the stencil $\mathcal{A} \subset \mathbb{Z}^d$ is finite. We define the symbol of L_ε as¹

$$(2.2) \quad l_\varepsilon(x, \zeta) = \sum_{\mu \in \mathcal{A}} l_\varepsilon(x, \mu) e^{i2\pi \varepsilon \mu \cdot \zeta}$$

for any $\zeta \in \mathbb{Z}^d$. By definition, we have

$$\left(L_\varepsilon e^{ix \cdot (\zeta_j b_j)} \right)(x) = l_\varepsilon(x, \zeta) e^{ix \cdot (\zeta_j b_j)}.$$

We choose \mathcal{A} as the minimal stencil, that is, for $\mu \in \mathcal{A}$, the symbol $l_\varepsilon(x, \mu)$ is not identically zero. For this choice of \mathcal{A} , we let

$$\underline{\mu}_i = \min_{\mu \in \mathcal{A}} \mu_i, \quad \bar{\mu}_i = \max_{\mu \in \mathcal{A}} \mu_i, \quad i = 1, \dots, d,$$

and call $(\underline{\mu}_i, \bar{\mu}_i)$ the *extent* of the difference operator in x_i direction.

2.2. Elliptic difference system. Consider a half-space

$$\Omega_{\text{half}} = \left\{ x a_1 + \sum_j y_j a_{j+1} \mid x \geq 0, y \in [0, 1)^{d-1} \right\}$$

with periodic boundary condition in y . Ω_{half} is discretized by grid points (x_ν, y_μ) with mesh size $\varepsilon = 1/(2N)$. Here $x_\nu = \varepsilon \nu a_1$ with $\nu \geq 0$ and $y_\mu = \varepsilon \sum_j \mu_j a_{j+1}$ with $\mu \in \mathbb{Z}^{d-1}$.

Consider a linear system of difference equations

$$(2.3) \quad \sum_{j=1}^n (L_{\varepsilon, ij} u_j)(x_\nu, y_\mu) = f_i(x_\nu, y_\mu), \quad i = 1, \dots, n$$

with boundary conditions

$$(2.4) \quad \sum_{j=1}^n (B_{\varepsilon, kj} u_j)(x_0, y_\mu) = \phi_k(y_\mu), \quad k = 1, \dots, q.$$

We denote $l_{\varepsilon, ij}$ the symbol of $L_{\varepsilon, ij}$ and $b_{\varepsilon, kj}$ the symbol of $B_{\varepsilon, kj}$ viewed as difference operators on the whole space, defined as in (2.2). For our purpose, it suffices to consider the case that the coefficients of difference operators are independent of x , y , and ε , *i.e.*,

$$l_{\varepsilon, ij}(x, y, \nu, \mu) = l_{ij}(\nu, \mu), \quad b_{\varepsilon, kj}(y, \nu, \mu) = b_{kj}(\nu, \mu).$$

We will henceforth make this simplification. Note that the symbols $l_{\varepsilon, ij}$ and $b_{\varepsilon, kj}$ however still depend on ε .

Definition 2.1 (Regular elliptic difference system). We call (2.3) a regular elliptic of order (σ, τ) for $\sigma, \tau \in \mathbb{Z}^n$ if the following conditions are satisfied.

i) For each $i, j = 1, \dots, n$ and ε sufficiently small,

$$|l_{\varepsilon, ij}(\zeta)| \lesssim \Lambda_\varepsilon(\zeta)^{\sigma_i + \tau_j};$$

¹To be consistent with [20], our scaling of the reciprocal space in terms of ε is slightly different from that of [28].

ii) There exist positive constants ζ_0 and ε_0 such that

$$|\det l_\varepsilon(\zeta)| \gtrsim \Lambda_\varepsilon(\zeta)^{2p}$$

for all $0 < \varepsilon \leq \varepsilon_0$ and $|\zeta| \geq \zeta_0$, where $2p = \sum_i (\sigma_i + \tau_i)$.

As a convention, we will choose σ and τ so that $\max \sigma_i = 0$.

We also take $\rho \in \mathbb{Z}^q$ so that

$$(2.5) \quad |b_{\varepsilon, kj}(\zeta)| \lesssim \Lambda_\varepsilon(\zeta)^{\rho_k + \tau_j},$$

and ρ_k is the smallest possible integer satisfying (2.5). (ρ, τ) gives the order of B_ε viewing as difference operators on the whole space.

We will assume that the operators $L_{\varepsilon, ij}$ and $B_{\varepsilon, kj}$ only contain differences of order $\sigma_i + \tau_j$ and $\rho_k + \tau_j$ respectively.

Assumption 1. Let the difference operators $L_{\varepsilon, ij}$ have extent $(\underline{\nu}_{ij}, \overline{\nu}_{ij})$ in x -direction, we assume that there are α^+, β^+ in \mathbb{Z}^d such that

$$0 \leq \underline{\nu}_{ij} \leq \overline{\nu}_{ij} \leq \alpha_i^+ + \beta_j^+, \quad i, j = 1, \dots, n,$$

and such that the number of roots $z(\eta)$, counting multiplicity, of the equation $R(z, \eta) = 0$ is $\sum_i (\alpha_i^+ + \beta_i^+)$. Here

$$\begin{aligned} R(z, \eta) &= \det \left[\sum_{\nu \in \mathbb{Z}} \sum_{\mu \in \mathbb{Z}^{d-1}} l_{ij}(\nu, \mu) z^\nu e^{i\mu \cdot \eta} \right] \\ &= \det [l_{\varepsilon, ij}(-i\varepsilon^{-1} \log z, \varepsilon^{-1} \eta)]. \end{aligned}$$

Furthermore, the number of boundary conditions q is equal to the number of roots of $R(z, \eta) = 0$ which satisfy

$$0 < |z(\eta)| < 1 \quad \text{for } |\eta| \neq 0.$$

In the case where q is larger than p , we need an additional assumption. We assume that the boundary conditions are ordered so that ρ_k are in increasing order. We define

$$\bar{\rho} = \max_{1 \leq k \leq p} (\rho_k + 1, 0),$$

and

$$\rho^* = \begin{cases} \min_{k > p} \rho_k + 1, & \text{if } q > p; \\ \infty, & \text{if } q = p. \end{cases}$$

Assumption 2. We assume that the boundary operators satisfy $\rho_k \geq \bar{\rho}$ for $p < k \leq q$.

In the limit $\varepsilon \rightarrow 0$, we obtain from the system of differential equations associated with the system of difference equations.

$$\begin{aligned} \sum_{j=1}^n (L_{ij}(\partial_x, \partial_y)u_j)(x, y) &= f_i(x, y) & i = 1, \dots, n, \\ \sum_{j=1}^n (B_{kj}(\partial_x, \partial_y)u_j)(0, y) &= \phi_k(y) & k = 1, \dots, p. \end{aligned}$$

The symbol of L_{ij} , denoted as $l_{ij}(\zeta)$, is given by

$$l_{ij}(\zeta) = \lim_{\varepsilon \rightarrow 0} l_{\varepsilon, ij}(\zeta).$$

We will make the following assumption on the symbol $l_{ij}(\zeta)$.

Assumption 3 (Supplementary condition). The determinant $\det[l_{ij}(\zeta)]$ is of even degree $2p$. For every pair of vectors $\zeta, \zeta' \in \mathbb{R}^d$, the polynomial $\det[l_{ij}(\zeta + \tau\zeta')]$ in the complex variable τ has exactly p roots with positive imaginary part.

Let G be the tangential grid given by

$$G = \{y_\mu \mid 0 \leq \mu_j < 2N, j = 1, \dots, d-1\}.$$

We define discrete Fourier transform for lattice functions u with respect to y as

$$\widehat{u}(x_\nu, \eta) = \left(\frac{\varepsilon}{2\pi}\right)^{d-1} \sum_{y_\mu \in G} e^{-i2\pi\varepsilon\eta \cdot \mu} u(x_\nu, y_\mu),$$

for $\eta \in \mathbb{Z}^{d-1}$ with $|\eta_j| \leq N$ for $j = 1, \dots, d-1$.

We define the following norms

$$\|u_j\|_{s, \varepsilon}^2 = \frac{\varepsilon}{2\pi} \sum_{\eta \in \mathbb{L}_{y, \varepsilon}^*} \sum_{\nu=0}^{\infty} \sum_{m=0}^{\lfloor s \rfloor} |\Lambda_\varepsilon(\eta)^{s-m} D_{x, \varepsilon}^m \widehat{u}_j(x_\nu, \eta)|^2,$$

and

$$\|u\|_{s+\tau, \varepsilon}^2 = \sum_{j=1}^d \|u_j\|_{s+\tau_j, \varepsilon}^2.$$

At the boundary, we define

$$|u_j|_{s, \varepsilon}^2 = \sum_{\eta \in \mathbb{L}_{y, \varepsilon}^*} \sum_{m=0}^{\lfloor s \rfloor} |\Lambda_\varepsilon(\eta)^{s-m} D_{x, \varepsilon}^m \widehat{u}_j(x_0, \eta)|^2,$$

and

$$|u|_{s+\tau, \varepsilon}^2 = \sum_{j=1}^d |u_j|_{s+\tau_j, \varepsilon}^2.$$

2.3. Complementing boundary condition. Due to periodicity in y , we may reduce the system to a one dimensional operator by Fourier transform. Recall that

$$L_{\varepsilon,ij} = \sum_{\nu \geq 0, \mu \in \mathbb{Z}^{d-1}} l_{ij}(\nu, \mu) T_{\varepsilon,x}^{\nu} T_{\varepsilon,y}^{\mu}.$$

Define coefficients $\tilde{l}_{\varepsilon,ij}$ for $\eta \in \mathbb{Z}^{d-1}$ as

$$\tilde{l}_{\varepsilon,ij}(\nu, \eta) = \sum_{\mu \in \mathbb{Z}^{d-1}} l_{ij}(\nu, \mu) e^{i2\pi\varepsilon\mu \cdot \eta}.$$

The reduced operator is given by

$$\tilde{L}_{\varepsilon,ij}(\eta) = \sum_{\nu \in \mathbb{Z}} \tilde{l}_{\varepsilon,ij}(\nu, \eta) T_{\varepsilon}^{\nu}.$$

Analogously, we define $\tilde{B}_{\varepsilon,kj}$ as the reduced operator of $B_{\varepsilon,kj}$. We denote $\tilde{B}_{\varepsilon}^1$ the operators corresponding to the first p boundary conditions and $\tilde{B}_{\varepsilon}^2$ for the remaining $q - p$ ones.

Similarly, we define the reduced operator for differential operators L_{ij} as

$$\tilde{L}_{ij}(\partial_x, \theta) = L_{ij}(\partial_x, i\theta)$$

for $\theta \in S^d$, and analogously for B_{kj} .

For the reduced operators, we consider three types of eigensolutions, which are defined as follows.

Definition 2.2. We call an eigensolution of type I a nontrivial solution of

$$(\tilde{L}_{\varepsilon}(\eta)w)(x_{\nu}) = 0 \quad \text{for some } \eta \neq 0,$$

satisfying

- (a) $(\tilde{B}_{\varepsilon}^1(\eta)w)(x_0) = 0;$
- (b) $(\tilde{B}_{\varepsilon}^2(\eta)w)(x_0) = 0;$
- (c) $w(x_{\nu}) \rightarrow 0$ as $\nu \rightarrow \infty.$

Definition 2.3. We call an eigensolution of type II a nontrivial solution of

$$(\tilde{L}(\partial_x, \theta)w)(x) = 0, \quad \text{for some } \theta \in S^d,$$

satisfying

- (a) $(\tilde{B}^1(\partial_x, \theta)w)(x_0) = 0;$
- (b) $w(x) \rightarrow 0$ as $x \rightarrow \infty.$

Definition 2.4. We call an eigensolution of type III a nontrivial solution to

$$(\tilde{L}_{\varepsilon}(0)w)(x) = 0,$$

satisfying

- (a) $(\tilde{B}_\varepsilon^2(0)w)(x_0) = 0;$
- (b) $w(x_\nu) \rightarrow 0$ as $\nu \rightarrow \infty$.

Remark. We remark that type I and type III eigensolutions are connected to the notion of surface phonon in the physics literature. The complementing conditions give a mathematical characterization of the surface phonon. On the other hand, the type II eigensolutions are surface waves at the boundary of the PDE.

Definition 2.5 (COMPLEMENTING BOUNDARY CONDITION). The system (2.3) with boundary conditions (2.4) satisfies the *Complementing Boundary Condition* if there are no eigensolutions of type I, II, or III.

The main result of [28, Theorem 3.1] is the following regularity estimate of the solution of elliptic system with boundary conditions.

Theorem 2. *If u is a solution to the system (2.3) with boundary conditions (2.4) and Assumptions 1, 2, and 3 are satisfied, then the following regularity estimate holds for each s with $\bar{\rho} \leq s < \rho^*$ and ε sufficiently small, if and only if, the Complementing Boundary Condition holds.*

$$(2.6) \quad \|u\|_{\tau+s,\varepsilon}^2 + |u|_{\tau+s-1/2,\varepsilon}^2 \lesssim |\phi_1|_{s-\rho-1/2,\varepsilon}^2 + \left| \varepsilon^{\rho-t+1/2} \phi_2 \right|_{s-t,\varepsilon}^2 + \|f\|_{s-\sigma,\varepsilon}^2 + \|u\|_{0,\varepsilon}^2,$$

where $t = \bar{\rho} + \frac{1}{2} \lfloor 2(s - \bar{\rho}) \rfloor$.

3. REGULARITY ESTIMATE FOR HYBRID SCHEMES

In this section we will apply the regularity estimate Theorem 2 to atomistic-to-continuum hybrid schemes.

We consider domain

$$\Omega_{\text{strip}} = \left\{ xa_1 + \sum_j y_j a_{j+1} \mid x \in \mathbb{R}, y \in [0, 1)^{d-1} \right\}$$

with periodic boundary condition in y variable. Ω_{strip} is discretized by grid points (x_ν, y_μ) with $x_\nu = \varepsilon \nu a_1$ with $\nu \in \mathbb{Z}$ and $y_\mu = \varepsilon \sum_j \mu_j a_{j+1}$ with $\mu \in \mathbb{Z}^{d-1}$. We consider the following hybrid system on Ω_{strip} :

$$(3.1) \quad \sum_{j=1}^d (\mathcal{H}_{\varepsilon,ij} u_j)(x_\nu, y_\mu) = f_i(x_\nu, y_\mu), \quad \nu < 0, \ i = 1, \dots, d;$$

$$(3.2) \quad \sum_{j=1}^d (\mathcal{H}_{\text{at},ij} u_j)(x_\nu, y_\mu) = f_i(x_\nu, y_\mu), \quad \nu \geq 0, \ i = 1, \dots, d.$$

We will reformulate the hybrid scheme as a system of difference equations with boundary conditions by folding with respect to the surface $\{x = 0\}$ (similar folding

trick was used in [7]). Let $(\underline{\nu}_{ij}^c, \overline{\nu}_{ij}^c)$ and $(\underline{\nu}_{ij}^a, \overline{\nu}_{ij}^a)$ be the extent of $\mathcal{H}_{\varepsilon,ij}$ and $\mathcal{H}_{\text{at},ij}$ in x direction respectively. To simplify the presentation, we will assume that the extents are the same for all i, j 's, which is usually the case for applications in atomistic-continuum hybrid schemes. We denote them as $(\underline{\nu}^c, \overline{\nu}^c)$ and $(\underline{\nu}^a, \overline{\nu}^a)$. The construction can be extended to more general cases, which will be omitted for simplicity. Without loss of generality, we also assume that $\underline{\nu}^a \leq \underline{\nu}^c \leq 0 \leq \overline{\nu}^c \leq \overline{\nu}^a$.

Let us rename the variables as

$$\begin{aligned} U_i(x_\nu, y_\mu) &= u_i(x_{\overline{\nu}^c - \nu - 1}, y_\mu), & \nu \geq 0, \mu \in \mathbb{R}^{d-1}; \\ U_{d+i}(x_\nu, y_\mu) &= u_i(x_{\underline{\nu}^a + \nu}, y_\mu), & \nu \geq 0, \mu \in \mathbb{R}^{d-1}. \end{aligned}$$

This leads to $d(\overline{\nu}^c - \underline{\nu}^a)$ compatibility conditions

$$(3.3) \quad U_i(x_\nu, y_\mu) = U_{d+i}(x_{\overline{\nu}^c - \underline{\nu}^a - \nu - 1}, y_\mu), \quad 0 \leq \nu \leq \overline{\nu}^c - \underline{\nu}^a - 1, i = 1, \dots, d.$$

We will rewrite equations (3.1)-(3.2) in terms of U 's. Define

$$L_{\varepsilon,ij} = \begin{cases} \sum_{0 \leq \nu \leq \overline{\nu}^c - \underline{\nu}^c, \mu} h_{\varepsilon,ij}(\overline{\nu}^c - \nu, \mu) T_{\varepsilon,x}^\nu T_{\varepsilon,y}^\mu, & i, j = 1, \dots, d; \\ \sum_{0 \leq \underline{\nu}^a \leq \nu \leq \overline{\nu}^a, \mu} h_{\text{at},(i-d)(j-d)}(\nu, \mu) T_{\varepsilon,x}^\nu T_{\varepsilon,y}^\mu, & i, j = d+1, \dots, 2d; \\ 0, & \text{otherwise.} \end{cases}$$

By construction, the extents of the operators L_ε are given by

$$(\underline{\nu}_{ij}, \overline{\nu}_{ij}) = \begin{cases} (0, \overline{\nu}^c - \underline{\nu}^c), & i, j = 1, \dots, d; \\ (0, \overline{\nu}^a - \underline{\nu}^a), & i, j = d+1, \dots, 2d; \\ (0, 0), & \text{otherwise.} \end{cases}$$

Let

$$F_i(x_\nu, y_\mu) = \begin{cases} f_i(x_{-\nu-1}, y_\mu), & i = 1, \dots, d; \\ f_{i-d}(x_\nu, y_\mu), & i = d+1, \dots, 2d, \end{cases}$$

we then have

$$(3.4) \quad \sum_{j=1}^{2d} (L_{\varepsilon,ij} U_j)(x_\nu, y_\mu) = F_i(x_\nu, y_\mu), \quad \nu \geq 0, \mu \in \mathbb{Z}^{d-1}.$$

We further define for $k = 1, \dots, d(\overline{\nu}^c - \underline{\nu}^a)$ and $j = 1, \dots, d$,

$$B_{\varepsilon,kj} = (D_{\varepsilon,e_1}^+)^i I \delta_{jl}, \quad B_{\varepsilon,k(j+d)} = -(D_{\varepsilon,-e_1}^+)^i T_{\varepsilon,x}^{\overline{\nu}^c - \underline{\nu}^a - 1} \delta_{jl},$$

where $i = \lfloor (k-1)/d \rfloor$ and $l = [(k-1) \bmod d] + 1$. The compatibility conditions (3.3) are then equivalent to the boundary conditions

$$(3.5) \quad \sum_{j=1}^{2d} (B_{\varepsilon,kj} U_j)(x_0, y_\mu) = 0, \quad \mu \in \mathbb{Z}^{d-1}, k = 1, \dots, d(\overline{\nu}^c - \underline{\nu}^a).$$

Therefore, we have reformulated (3.1)-(3.2) into a difference system (3.4) with boundary conditions (3.5).

Since

$$(3.6) \quad |\det l_{\varepsilon,ij}(\zeta)| = |\det h_{\varepsilon,ij}(\zeta)| |\det h_{\text{at},ij}(\zeta_2)|.$$

The regular ellipticity of the operator L_ε is guaranteed by Assumption A, as \mathcal{H}_{at} and \mathcal{H}_ε are both regular elliptic by Lemma 1.1. Moreover, the order of L_ε is $(2, 0)$, and hence, $p = 2d$.

Taking $\alpha^+ = 0$, $\beta_j^+ = \overline{\nu}^c - \underline{\nu}^c$, $j = 1, \dots, d$, and $\beta_j^+ = \overline{\nu}^a - \underline{\nu}^a$, $j = d+1, \dots, 2d$, we have then $0 \leq \underline{\nu}_{ij} \leq \overline{\nu}_{ij} \leq \alpha_i^+ + \beta_j^+$. The number of boundary conditions we have imposed on (3.5) is $q = d(\overline{\nu}^c - \underline{\nu}^a)$. Define

$$\begin{aligned} R^c(z, \eta) &= \det [h_{\varepsilon,ij}(-i\varepsilon^{-1} \log z, \varepsilon^{-1}\eta)]; \\ R^a(z, \eta) &= \det [h_{\text{at},ij}(-i\varepsilon^{-1} \log z, \varepsilon^{-1}\eta)]. \end{aligned}$$

From (3.6), the Assumption 1 for the system (3.4)-(3.5) is equivalent to

Assumption B. The number of boundary conditions $d(\overline{\nu}^c - \underline{\nu}^a)$ is equal to the total number of roots of $R^c(z, \eta) = 0$ and $R^a(z, \eta) = 0$ which satisfy

$$0 < |z(\eta)| < 1 \quad \text{for } |\eta| \neq 0.$$

We remark that this assumption is satisfied for linearized finite difference operators given by common inter-atomic potentials.

By definition, we have

$$\rho_k = \lfloor (k-1)/d \rfloor - 2.$$

Hence, $\bar{\rho} = 0$ and $\rho^* = 1$. Assumption 2 is satisfied by the system (3.4)-(3.5).

The Supplementary Assumption 3 is automatically satisfied since $2d \geq 3$ as a result in [2].

The stability of the hybrid scheme relies on the stability at interface, which is characterized by the complementing boundary condition.

Assumption C. The hybrid system (3.1)-(3.2), or equivalently (3.4)-(3.5) satisfies the *Complementing Boundary Condition*, i.e., there are no eigensolutions of type I, II, or III.

This stability assumption needs to be check for particular atomic interaction potentials. We will discuss an example in Section 5.

We can now state the regularity estimate for the hybrid system (3.1)-(3.2).

Proposition 3.1 (Regularity). *If u is a solution of the system (3.1)-(3.2), under Assumptions A, B, and C, the following regularity estimate holds for ε sufficiently small*

$$(3.7) \quad \|u\|_{2,\varepsilon} \lesssim \|f\|_{0,\varepsilon} + \|u\|_{0,\varepsilon}.$$

Proof. Applying Theorem 2 to the system (3.4) with boundary conditions (3.5), we have

$$\|U\|_{2,\varepsilon} \lesssim \|F\|_{0,\varepsilon} + \|U\|_{0,\varepsilon}.$$

By definition of F and U , it is clear that $\|F\|_{0,\varepsilon} = \|f\|_{0,\varepsilon}$, $\|U\|_{0,\varepsilon} \leq 2\|u\|_{0,\varepsilon}$, and $\|u\|_{2,\varepsilon} \leq \|U\|_{2,\varepsilon}$. Therefore, we obtain

$$\|u\|_{2,\varepsilon} \lesssim \|f\|_{0,\varepsilon} + \|u\|_{0,\varepsilon}.$$

This completes the proof. \square

The regularity estimate for the linearized operator $\mathcal{H}_{\text{hy}} = \mathcal{H}_{\text{hy}}[0]$ then follows.

Theorem 3 (Regularity). *Under Assumptions A, B, and C, for any $v \in H_\varepsilon^2(\Omega)$, we have*

$$(3.8) \quad \|v\|_{2,\varepsilon} \lesssim \|\mathcal{H}_{\text{hy}}v\|_{0,\varepsilon} + \|v\|_{0,\varepsilon}$$

for ε sufficiently small.

Proof. The theorem follows from Proposition 3.1 combined with a standard localization argument as in [18]. We sketch the proof here for completeness.

Let φ_1 and φ_2 be a partition of unity of the domain Ω , such that $\varphi_1, \varphi_2 \in C^\infty(\Omega)$, $\varphi_1 + \varphi_2 = 1$, $\varphi_1(x) = 1$ if $x_1 \in [3/8, 5/8]$, and $\varphi_1(x) = 0$ if $x_1 \in [0, 1/8) \cup [7/8, 1]$. We then have

$$\|v\|_{2,\varepsilon} \leq \|\varphi_1v\|_{2,\varepsilon} + \|\varphi_2v\|_{2,\varepsilon}.$$

The estimates for the two terms on the right hand side are the same, we only consider $\|\varphi_1v\|_{2,\varepsilon}$ in the following. Let $u = \varphi_1v$, since φ_1 is compactly supported in Ω , we can extend u by 0 as a function on the grid points in Ω_{strip} . Note that

$$\|\mathcal{H}_{\text{hy}}u\|_{0,\varepsilon} = \|\mathcal{H}_{\text{hy}}(\varphi_1v)\| \lesssim \|\mathcal{H}_{\text{hy}}v\|_{2,\varepsilon} + \|v\|_{0,\varepsilon},$$

since φ_1 is a smooth function. Thus, by Proposition 3.1, we have

$$\|\varphi_1v\|_{2,\varepsilon} \lesssim \|\mathcal{H}_{\text{hy}}u\|_{0,\varepsilon} + \|u\|_{0,\varepsilon} \lesssim \|\mathcal{H}_{\text{hy}}v\|_{2,\varepsilon} + \|v\|_{0,\varepsilon}.$$

Therefore, we obtain the regularity estimate (3.8). \square

4. STABILITY

The main theorem in this section is the following stability estimate.

Theorem 4 (Stability). *Under Assumptions A, B, and C, for any $v \in H_\varepsilon^2(\Omega)$ with mean zero, we have*

$$(4.1) \quad \|v\|_{\varepsilon,2} \lesssim \|\mathcal{H}_{\text{hy}}v\|_{\varepsilon,0}$$

for ε sufficiently small.

To obtain the stability estimate from the regularity estimate Theorem 3, we need to eliminate $\|v\|_{\varepsilon,0}$ on the right hand side of (3.8). The proof is based on the uniqueness of the continuous system from ellipticity, the consistency of the finite difference schemes to the continuous system, and the regularity estimate Theorem 3. We remark that the stability analysis in our previous work [20] relies on the smoothness of ϱ , so it does not apply to the sharp transition case. The current proof does not require smoothness of ϱ and so applies both to the hybrid method with smooth or sharp transitions.

In order to connect the finite difference system with continuous PDE, we need to extend grid functions on Ω_ε to continuous functions defined in Ω . For this purpose, let us define an interpolation operator Q_ε as follows. For any lattice function u on Ω_ε , we define $Q_\varepsilon u \in L^2(\Omega)$ as

$$(4.2) \quad (Q_\varepsilon u)(x) = \sum_{\xi \in \mathbb{L}_\varepsilon^*} e^{ix \cdot \xi} \widehat{u}(\xi), \quad x \in \Omega.$$

Comparing with (1.2), we know that $Q_\varepsilon u$ agrees with u on Ω_ε . We have the following properties of Q_ε .

Lemma 4.1. *For $k \geq 0$, there exists constants $c_k, C_k > 0$, such that for any u ,*

$$c_k \|u\|_{H_\varepsilon^k(\Omega)} \leq \|Q_\varepsilon u\|_{H^k(\Omega)} \leq C_k \|u\|_{H_\varepsilon^k(\Omega)}.$$

Proof. It is not hard to check for any $\xi \in \mathbb{L}_\varepsilon^*$, it holds

$$c\Lambda^2(\zeta) \leq \Lambda_\varepsilon^2(\zeta) \leq \Lambda^2(\zeta).$$

The conclusion follows. \square

Let χ be a standard nonnegative cut-off function on \mathbb{R}^d , which is smooth and compactly supported, with $\|\chi\|_{L^1} = 1$. Let χ_ε be the scaled version

$$\chi_\varepsilon(x) = \varepsilon^{-(\alpha d)} \chi(\varepsilon^{-\alpha} x),$$

for some α with $0 < \alpha < 1$. The choice of the value of α will be specified in the proof of Proposition 4.4.

Define a low-pass filter operator K_ε for $f \in L^2(\Omega)$ using $\widehat{\chi}_\varepsilon$ as Fourier multiplier:

$$\widehat{K_\varepsilon f}(\xi) = (2\pi)^d \widehat{f}(\xi) \widehat{\chi}_\varepsilon(\xi) = (2\pi)^d \widehat{f}(\xi) \widehat{\chi}(\varepsilon^\alpha \xi).$$

In real space, K_ε convolves f with χ_ε . Integrating by parts, we obtain

$$(4.3) \quad |\widehat{\chi}_\varepsilon(\xi)| \leq C_k |\varepsilon^\alpha \xi|^{-k}, \quad \text{for all } k \in \mathbb{Z}_+,$$

$$(4.4) \quad (2\pi)^d \widehat{\chi}_\varepsilon(0) = 1.$$

Hence, K_ε is indeed a low-pass filter. For simplicity of notation, we denote

$$\bar{u}_\varepsilon = K_\varepsilon Q_\varepsilon u_\varepsilon,$$

for lattice function u_ε on Ω_ε .

Let us first recall some consistency results proved in [20, Section 2] (proofs of these results do not depend on the smoothness of ϱ), which will be used in the proof of stability below.

Lemma 4.2 (Consistency). *For any u smooth, we have*

$$(4.5) \quad \|\mathcal{F}_{\text{at}}[u] - \mathcal{F}_{\text{CB}}[u]\|_{L_\varepsilon^\infty} \leq C\varepsilon^2 \|u\|_{W^{18,\infty}},$$

$$(4.6) \quad \|\mathcal{F}_\varepsilon[u] - \mathcal{F}_{\text{CB}}[u]\|_{L_\varepsilon^\infty} \leq C\varepsilon^2 \|u\|_{W^{18,\infty}},$$

and

$$(4.7) \quad \|\mathcal{F}_{\text{hy}}[u] - \mathcal{F}_{\text{at}}[u]\|_{L_\varepsilon^\infty} \leq C\varepsilon^2 \|u\|_{W^{18,\infty}},$$

where the constant C depends on V and $\|u\|_{L^\infty}$, but is independent of ε .

Using Lemma 4.2, we prove the consistency results for linearized operators.

Lemma 4.3 (Consistency of symbols of linearized operators). *There exists $\varepsilon_0 > 0$ and $s > 0$ such that for any $\varepsilon \leq \varepsilon_0$, $x \in \Omega_\varepsilon$, and $\xi \in \mathbb{L}_\varepsilon^*$, we have*

$$(4.8) \quad |h_{\text{at}}(\xi) - h_{\text{CB}}(\xi)| \leq C\varepsilon^2(1 + |\xi|^2)^{s/2},$$

$$(4.9) \quad |h_{\text{at}}(\xi) - h_{\text{hy}}(x, \xi)| \leq C\varepsilon^2(1 + |\xi|^2)^{s/2}.$$

Proof. The proof for (4.8) and (4.9) are analogous, and hence we will only prove the latter. By definition, for $1 \leq j, k \leq d$,

$$\begin{aligned} (h_{\text{at}})_{jk}(\xi) &= e^{-ix \cdot \xi} (\mathcal{H}_{\text{at}}(e_k f_\xi))_j(x), \\ (h_{\text{hy}})_{jk}(x, \xi) &= e^{-ix \cdot \xi} (\mathcal{H}_{\text{hy}}(e_k f_\xi))_j(x). \end{aligned}$$

where $f_\xi(x) = e^{ix \cdot \xi}$ for $x \in \Omega$. Taking difference of the above two equations, we obtain the bound

$$|h_{\text{at}}(\xi) - h_{\text{hy}}(x, \xi)| \leq C \sup_{1 \leq k \leq d} \|\mathcal{H}_{\text{at}}(e_k f_\xi) - \mathcal{H}_{\text{hy}}(e_k f_\xi)\|_{L_\varepsilon^\infty}.$$

Note that by the definition of linearized operators \mathcal{H}_{at} and \mathcal{H}_{hy} , we have

$$\mathcal{H}_{\text{at}}(e_k f_\xi) - \mathcal{H}_{\text{hy}}(e_k f_\xi) = \lim_{t \rightarrow 0^+} \frac{1}{t} (\mathcal{F}_{\text{at}}[t(e_k f_\xi)] - \mathcal{F}_{\text{hy}}[t(e_k f_\xi)]).$$

Hence,

$$\begin{aligned} \|\mathcal{H}_{\text{at}}(e_k f_\xi) - \mathcal{H}_{\text{hy}}(e_k f_\xi)\|_{L_\varepsilon^\infty} &= \lim_{t \rightarrow 0^+} \frac{1}{t} \|\mathcal{F}_{\text{at}}[t(e_k f_\xi)] - \mathcal{F}_{\text{hy}}[t(e_k f_\xi)]\|_{L_\varepsilon^\infty} \\ &\lesssim \varepsilon^2 \|e_k f_\xi\|_{W^{18,\infty}} \lesssim \varepsilon^2 \|e_k f_\xi\|_{H^s} \lesssim \varepsilon^2 (1 + |\xi|^2)^{s/2}, \end{aligned}$$

where s is chosen so that the Sobolev inequality $\|f\|_{W^{18,\infty}(\Omega)} \leq C \|f\|_{H^s(\Omega)}$ holds for any $f \in H^s(\Omega)$ (s depends on the dimension). Here, we have used Lemma 4.2 in the first inequality, noticing that $\|te_k f_\xi\|_{L^\infty}$ is uniformly bounded for ξ as $t \rightarrow 0$. This concludes the proof. \square

With these preparations, we now state a key proposition will be used in the proof of Theorem 4.

Proposition 4.4. *For $\{v_\varepsilon\}_{\varepsilon>0}$ such that $v_\varepsilon \in H_\varepsilon^2(\Omega)$ and $\|v_\varepsilon\|_{\varepsilon,2}$ is uniformly bounded, we have*

$$\lim_{\varepsilon \rightarrow 0+} \|\mathcal{H}_{\text{CB}} \bar{v}_\varepsilon - \overline{\mathcal{H}_{\text{hy}} v_\varepsilon}\|_{L^2(\Omega)} = 0.$$

Proof. By triangular inequality,

$$\begin{aligned} \|\mathcal{H}_{\text{CB}} \bar{v}_\varepsilon - \overline{\mathcal{H}_{\text{hy}} v_\varepsilon}\|_{L^2(\Omega)} &\leq \|\overline{\mathcal{H}_{\text{hy}} \bar{v}_\varepsilon} - \overline{\mathcal{H}_{\text{hy}} v_\varepsilon}\|_{L^2(\Omega)} + \|\overline{\mathcal{H}_{\text{at}} \bar{v}_\varepsilon} - \overline{\mathcal{H}_{\text{hy}} \bar{v}_\varepsilon}\|_{L^2(\Omega)} \\ &\quad + \|\mathcal{H}_{\text{CB}} \bar{v}_\varepsilon - \overline{\mathcal{H}_{\text{at}} \bar{v}_\varepsilon}\|_{L^2(\Omega)}. \end{aligned}$$

Hence, it suffices to show each term on the right-hand side goes to zero as $\varepsilon \rightarrow 0$.

Step 1. By Lemma 4.1 and the definition of \mathcal{H}_{hy} , we have

$$\begin{aligned} \|\overline{\mathcal{H}_{\text{hy}} \bar{v}_\varepsilon} - \overline{\mathcal{H}_{\text{hy}} v_\varepsilon}\|_{L^2(\Omega)} &\leq \|\mathcal{H}_{\text{hy}} \bar{v}_\varepsilon - \mathcal{H}_{\text{hy}} v_\varepsilon\|_{\varepsilon,0} \\ &\leq \|\mathcal{H}_{\text{at}} \bar{v}_\varepsilon - \mathcal{H}_{\text{at}} v_\varepsilon\|_{\varepsilon,0} + \|\mathcal{H}_\varepsilon \bar{v}_\varepsilon - \mathcal{H}_\varepsilon v_\varepsilon\|_{\varepsilon,0}. \end{aligned}$$

We now show that $\|\mathcal{H}_\varepsilon \bar{v}_\varepsilon - \mathcal{H}_\varepsilon v_\varepsilon\|_{\varepsilon,0}$ converges to zero as $\varepsilon \rightarrow 0$, the argument for the other term is identical. By Parseval's identity,

$$(4.10) \quad \|\mathcal{H}_\varepsilon \bar{v}_\varepsilon - \mathcal{H}_\varepsilon v_\varepsilon\|_{\varepsilon,0} = \|h_\varepsilon(\xi)(\widehat{\chi}_\varepsilon(\xi) - 1)\widehat{v}_\varepsilon(\xi)\|_{l^2(\mathbb{L}_\varepsilon^*)}.$$

Note that $\|h_\varepsilon(\xi)\widehat{v}_\varepsilon(\xi)\|_{l^2(\mathbb{L}_\varepsilon^*)} = \|\mathcal{H}_\varepsilon v_\varepsilon\|_{\varepsilon,0}$ is bounded as $v_\varepsilon \in H_\varepsilon^2(\Omega)$ and that $\widehat{\chi}_\varepsilon(\xi) \rightarrow 1$ for any $\xi \in \mathbb{L}_\varepsilon^*$, as $\varepsilon \rightarrow 0$. By dominance convergence, the right-hand side of (4.10) converges to zero in the limit. Therefore, $\|\overline{\mathcal{H}_{\text{hy}} \bar{v}_\varepsilon} - \overline{\mathcal{H}_{\text{hy}} v_\varepsilon}\|_{L^2(\Omega)} \rightarrow 0$.

Step 2. By Lemma 4.1, we have

$$\|\overline{\mathcal{H}_{\text{at}} \bar{v}_\varepsilon} - \overline{\mathcal{H}_{\text{hy}} \bar{v}_\varepsilon}\|_{L^2(\Omega)} \lesssim \|\mathcal{H}_{\text{at}} \bar{v}_\varepsilon - \mathcal{H}_{\text{hy}} \bar{v}_\varepsilon\|_{\varepsilon,0}.$$

Hence it suffices to estimate the right-hand side. We calculate

$$\mathcal{H}_{\text{at}} \bar{v}_\varepsilon - \mathcal{H}_{\text{hy}} \bar{v}_\varepsilon = \sum_{\xi \in \mathbb{L}_\varepsilon^*} (h_{\text{at}}(\xi) - h_{\text{hy}}(x, \xi)) \widehat{v}_\varepsilon(\xi) e^{ix \cdot \xi}.$$

Therefore, using (4.9) in Lemma 4.3, we have

$$\|\mathcal{H}_{\text{at}} \bar{v}_\varepsilon - \mathcal{H}_{\text{hy}} \bar{v}_\varepsilon\|_{\varepsilon,0}^2 \lesssim \sum_{\xi \in \mathbb{L}_\varepsilon^*} \varepsilon^4 (1 + |\xi|^2)^s |\widehat{v}_\varepsilon(\xi)|^2.$$

To estimate the right-hand side, note that by (4.3) we have for any $k \in \mathbb{Z}_+$,

$$|\widehat{v}_\varepsilon(\xi)|^2 = |\widehat{\chi}_\varepsilon(\xi)|^2 |\widehat{v}_\varepsilon(\xi)|^2 \leq C_k |\varepsilon^\alpha \xi|^{-2k} |\widehat{v}_\varepsilon(\xi)|^2.$$

Taking k sufficiently large so that $(1 + |\xi|^2)^s |\xi|^{-2k}$ is bounded for $\xi \in \mathbb{L}^* \setminus \{0\}$, we then have

$$\|\mathcal{H}_{\text{at}} \bar{v}_\varepsilon - \mathcal{H}_{\text{hy}} \bar{v}_\varepsilon\|_{\varepsilon,0}^2 \lesssim \varepsilon^4 \varepsilon^{-2\alpha k} \sum_{\xi \in \mathbb{L}_\varepsilon^*} |\widehat{v}_\varepsilon(\xi)|^2$$

Choosing α in the low-pass filter operator to satisfy

$$(4.11) \quad \alpha < 2/k$$

guarantees that $\|\overline{\mathcal{H}_{\text{at}}\bar{v}_\varepsilon} - \overline{\mathcal{H}_{\text{hy}}\bar{v}_\varepsilon}\|_{L^2(\Omega)} \rightarrow 0$ as $\varepsilon \rightarrow 0$.

Step 3. By definition,

$$\widehat{\mathcal{H}_{\text{CB}}\bar{v}_\varepsilon}(\xi) = h_{\text{CB}}(\xi)\widehat{\chi}(\varepsilon^\alpha\xi)\widehat{v}_\varepsilon(\xi).$$

For the discrete system, we have

$$\begin{aligned}\widehat{\mathcal{H}_{\text{at}}\bar{v}_\varepsilon}(\xi) &= \widehat{\chi}(\varepsilon^\alpha\xi)\left(\frac{\varepsilon}{2\pi}\right)^d \sum_{x \in \Omega_\varepsilon} e^{-i\xi \cdot x} \sum_{\eta \in \mathbb{L}_\varepsilon^*} e^{ix \cdot \eta} h_{\text{at}}(\eta) \widehat{v}_\varepsilon(\eta) \\ &= \widehat{\chi}(\varepsilon^\alpha\xi) h_{\text{at}}(\xi) \widehat{v}_\varepsilon(\xi).\end{aligned}$$

Hence, we have, combined with (4.8) and (4.3), for some $s > 0$ and any $k \in \mathbb{Z}_+$,

$$\begin{aligned}\|\mathcal{H}_{\text{CB}}\bar{v}_\varepsilon - \overline{\mathcal{H}_{\text{at}}\bar{v}_\varepsilon}\|_{L^2(\Omega)}^2 &= \sum_{\xi \in \mathbb{L}_\varepsilon^*} (h_{\text{at}}(\xi) - h_{\text{CB}}(\xi))^2 |\widehat{\chi}(\varepsilon^\alpha\xi)|^2 |\widehat{v}_\varepsilon(\xi)|^2 \\ &\leq C_k \varepsilon^4 \sum_{\xi \in \mathbb{L}_\varepsilon^*} (1 + |\xi|)^s |\varepsilon^\alpha\xi|^{-2k} |\widehat{v}_\varepsilon(\xi)|^2.\end{aligned}$$

We choose a sufficiently large k , so that the right hand side is bounded by $C\varepsilon^{4-2\alpha k} \|v_\varepsilon\|_{\varepsilon,0}^2$.

The choice of α in (4.11) guarantees that $\|\mathcal{H}_{\text{CB}}\bar{v}_\varepsilon - \overline{\mathcal{H}_{\text{at}}\bar{v}_\varepsilon}\|_{L^2(\Omega)} \rightarrow 0$ as $\varepsilon \rightarrow 0$. \square

Proof of Theorem 4. Suppose (4.1) does not hold, then there is a sequence of functions $\{w_k\}$ and $\varepsilon_k > 0$ such that

$$\begin{aligned}\|w_k\|_{\varepsilon_k,2} &\rightarrow \infty, & \text{as } k \rightarrow \infty; \\ \|\mathcal{H}_{\text{hy}}w_k\|_{\varepsilon_k,0} &\leq c, & \text{for all } k; \\ \sum_{x \in \Omega_{\varepsilon_k}} w_k(x) &= 0, & \text{for all } k.\end{aligned}$$

Set $v_k = w_k / \|w_k\|_{\varepsilon_k,2}$, we then have

$$(4.12) \quad \|v_k\|_{\varepsilon_k,2} = 1 \quad \text{for all } k;$$

$$(4.13) \quad \|\mathcal{H}_{\text{hy}}v_k\|_{\varepsilon_k,0} \rightarrow 0, \quad \text{as } k \rightarrow \infty;$$

$$(4.14) \quad \sum_{x \in \Omega_{\varepsilon_k}} v_k(x) = 0, \quad \text{for all } k.$$

Since

$$\mathcal{H}_{\text{CB}}\bar{v}_k = \overline{\mathcal{H}_{\text{hy}}v_k} + (\mathcal{H}_{\text{CB}}\bar{v}_k - \overline{\mathcal{H}_{\text{hy}}v_k}).$$

Since $\|\mathcal{H}_{\text{hy}}v_k\|_{\varepsilon_k,0} \rightarrow 0$, we have

$$\|\overline{\mathcal{H}_{\text{hy}}v_k}\|_{L^2(\Omega)} \rightarrow 0, \quad \text{as } k \rightarrow \infty.$$

Moreover, by Proposition 4.4,

$$\|\mathcal{H}_{\text{CB}}\bar{v}_k - \overline{\mathcal{H}_{\text{hy}}v_k}\|_{L^2(\Omega)} \rightarrow 0, \quad \text{as } k \rightarrow \infty.$$

Hence $\|\mathcal{H}_{\text{CB}}\bar{v}_k\|_{L^2(\Omega)} \rightarrow 0$. Note also that the average of \bar{v}_k is zero, since $\widehat{\bar{v}_k}(0) = 0$. By the invertibility of \mathcal{H}_{CB} on the subspace orthogonal to constant function,

$\|\bar{v}_k\|_{L^2(\Omega)} \rightarrow 0$, as $k \rightarrow \infty$, while $\|v_k\|_{\varepsilon_k,2} = 1$. It follows then $\|v_k\|_{\varepsilon_k,0} \rightarrow 0$. Indeed, since

$$\|v_k\|_{\varepsilon_k,1} = \sum_{\xi \in \mathbb{L}_{\varepsilon_k}^*} \Lambda_{\varepsilon_k}^2(\xi) |\widehat{v}_k(\xi)|^2 \leq 1,$$

for any $\delta > 0$, there exist $\Xi > 0$ and k_1 , such that for any $k \geq k_1$,

$$(4.15) \quad \sum_{\xi \in \mathbb{L}_{\varepsilon_k}^*, |\xi| \geq \Xi} |\widehat{v}_k(\xi)|^2 < \delta/2.$$

On the other hand, due to (4.4), there exists k_2 , such that for $k \geq k_2$

$$(4.16) \quad \sum_{\xi \in \mathbb{L}_{\varepsilon_k}^*, |\xi| < \Xi} \left| |\widehat{v}_k(\xi)|^2 - |\widehat{\bar{v}}_k(\xi)|^2 \right| \leq \delta/4.$$

Moreover, as $\|\bar{v}_k\|_{L^2} \rightarrow 0$, there exists k_3 , such that for $k \geq k_3$,

$$(4.17) \quad \sum_{\xi \in \mathbb{L}_{\varepsilon_k}^*, |\xi| < \Xi} |\widehat{\bar{v}}_k(\xi)|^2 \leq \delta/4.$$

Combined (4.15)–(4.17) together, we have for $k \geq \max(k_1, k_2, k_3)$,

$$\|v_k\|_{\varepsilon_k,0}^2 = \sum_{\xi \in \mathbb{L}_{\varepsilon_k}^*} |\widehat{v}_k(\xi)|^2 \leq \delta.$$

Hence, $\lim_{k \rightarrow \infty} \|v_k\|_{\varepsilon_k,0} = 0$. From Theorem 3, this implies

$$\lim_{k \rightarrow \infty} \|v_k\|_{\varepsilon_k,2} = 0.$$

The contradiction with the choice of v_k proves the Theorem. \square

Theorem 4 extends to a deformed state u , we omit the proof which is the same as [20, Theorem 4.6].

Theorem 5 (Stability). *Under Assumptions A, B, and C, there exists $\delta > 0$, such that for any $\varepsilon > 0$ and u , $\|u\|_{W_\varepsilon^{2,\infty}} \leq \delta$ and any $v \in H_\varepsilon^2(\Omega)$ with mean zero, we have*

$$(4.18) \quad \|v\|_{\varepsilon,2} \leq C \|\Pi_\varepsilon \mathcal{H}_{\text{hy}}[u]v\|_{\varepsilon,0},$$

where the constant depends on δ , but is independent of u , v and ε .

5. EXAMPLES

We apply the result here to a particular example of atomistic-to-continuum hybrid method. Consider a force-based method on a triangular lattice. Figure 1 gives the geometry and the choice of the atomistic and continuum regions. The interface between the atomistic and continuum regions is parallel to the $(1, \sqrt{3})/2$ direction of the lattice. The interaction between atoms is assumed to be harmonic (quadratic potential). The force balance equation reads

$$\Pi_\varepsilon \mathcal{F}_{\text{hy}}[y](x) = f_\varepsilon(x),$$

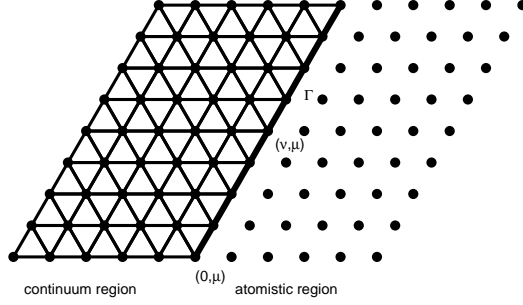


FIGURE 1. Illustration of the geometry and coupling interface of the hybrid method. The coordinate of each atom is (ν, μ) , and the interface Γ along the atoms labeled with $(0, \mu)$. The interface Γ divides the domain into the atomistic region Ω_a and the continuum region Ω_c .

where \mathcal{F}_{hy} is given by

$$\mathcal{F}_{\text{hy}}[z](x) = \begin{cases} \mathcal{F}_{\text{at}}[z](x), & x \in \Omega_a, \\ \mathcal{F}_{\varepsilon}[z](x), & x \in \Omega_c, \end{cases}$$

with

$$\begin{aligned} \mathcal{F}_{\text{at}}[z](x) &:= \frac{1}{\varepsilon^2} \sum_{i=1}^{12} [z(x + s_i) - z(x)], \\ \mathcal{F}_{\varepsilon}[z](x) &:= \frac{4}{\varepsilon^2} \sum_{i=1}^6 [z(x + s_i) - z(x)], \end{aligned}$$

where $\{s_i\}_{i=1}^{12}$ is the interaction range of the first and the second neighborhood interaction of the triangular lattice.

We rewrite the coupled force balance equation into a system. Define the map

$$Tx = (-x_1, x_2),$$

and denote

$$\tilde{y}(x) = y(Tx), \quad \text{and} \quad z(x) = (y(x), \tilde{y}(x)).$$

The hybrid method can be written as

$$(5.1) \quad \mathcal{F}_{\text{hy}}[z](x) = \ell_{\varepsilon}(x),$$

where

$$\mathcal{F}_{\text{hy}} = \begin{pmatrix} \mathcal{F}_{\text{at}} & 0 \\ 0 & \mathcal{F}_{\varepsilon} \end{pmatrix},$$

and $\ell_{\varepsilon}(x) = (f_{\varepsilon}(x), f_{\varepsilon}(Tx))$.

The equilibrium equations (5.1) are supplemented with the following boundary condition

$$(5.2) \quad z(x) = \mathcal{S}z(Tx) \quad \text{on} \quad \Gamma,$$

where Γ is the interface as shown in Figure 1 and

$$\mathcal{S} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

Applying Fourier transform in the tangential direction, we obtain

$$\begin{aligned} \tilde{\mathcal{F}}_\varepsilon &= \frac{4}{\varepsilon^2} (T_{s_1}(1 + e^{-i\xi \cdot s_2}) + T_{-s_1}(1 + e^{i\xi \cdot s_2}) + 2\cos(\xi \cdot s_2) - 6), \\ \tilde{\mathcal{F}}_{\text{at}} &= \frac{1}{\varepsilon^2} (T_{s_1}(1 + e^{-i\xi \cdot s_2} + e^{i\xi \cdot s_2} + e^{-2i\xi \cdot s_2}) + T_{-s_1}(1 + e^{i\xi \cdot s_2} + e^{-i\xi \cdot s_2} + e^{2i\xi \cdot s_2}) \\ &\quad + T_{2s_1}e^{-i\xi \cdot s_2} + T_{-2s_1}e^{i\xi \cdot s_2} + 2\cos(\xi \cdot s_2) - 12). \end{aligned}$$

The first step is to consider the distribution of the root of the following two characterization equations. Let $\zeta = e^{i\xi \cdot s_2} = e^{i\theta}$, obviously $\zeta \neq 1$ unless $\theta = 0$.

$$(5.3) \quad z(1 + \bar{\zeta}) + z^{-1}(1 + \zeta) + \zeta + \bar{\zeta} - 6 = 0,$$

and

$$(5.4) \quad \begin{aligned} &z^2\bar{\zeta} + z^{-2}\zeta + z(1 + \zeta + \bar{\zeta} + \bar{\zeta}^2) \\ &\quad + z^{-1}(1 + \zeta + \bar{\zeta} + \zeta^2) + \zeta + \bar{\zeta} - 12 = 0. \end{aligned}$$

The equation (5.3) can be written as

$$z^2 - \frac{6 - \zeta - \bar{\zeta}}{1 + \bar{\zeta}}z + \zeta = 0.$$

The roots z_1 and z_2 of the above equation satisfy $|z_1 z_2| = |\zeta| = 1$. We cannot have $|z_1| = |z_2| = 1$, otherwise $\det \tilde{\mathcal{F}}_\varepsilon = 0$, which contradicts with the bulk stability condition. Therefore, we have two distinct roots, one inside the unit disk, the other outside.

To deal with (5.4), we let $z = w\zeta^{1/2}$, and write (5.4) as

$$(5.5) \quad w^2 + w^{-2} + (\zeta^{1/2} + \bar{\zeta}^{1/2} + \zeta^{3/2} + \bar{\zeta}^{3/2})(w + w^{-1}) + \zeta + \zeta^{-1} - 12 = 0.$$

Let $s = w + w^{-1}$ and $A = \zeta^{1/2} + \bar{\zeta}^{1/2} + \zeta^{3/2} + \bar{\zeta}^{3/2}$, we write the above equation as

$$s^2 + As + \zeta + \bar{\zeta} - 14 = 0.$$

Denote by $f(s) = s^2 + As + \zeta + \bar{\zeta} - 14$. Note that

$$\begin{aligned} f(2) &= 2A + \zeta + \bar{\zeta} - 10 \\ &= 2(\zeta^{1/2} + \bar{\zeta}^{1/2} - 2) \left(\left(\zeta^{1/2} + \bar{\zeta}^{1/2} + 5/4 \right)^2 + \frac{23}{16} \right) \\ &\leq 0. \end{aligned}$$

It is clear that $f(2) < 0$ unless $\zeta = 1$, which is impossible. Proceeding along the same line, we obtain

$$\begin{aligned} f(-2) &= -2A + \zeta + \bar{\zeta} - 10 \\ &= -2(\zeta^{1/2} + \bar{\zeta}^{1/2} + 2) \left(\left(\zeta^{1/2} + \bar{\zeta}^{1/2} - 5/4 \right)^2 + \frac{23}{16} \right) \\ &< 0. \end{aligned}$$

We immediately have, there exists two roots s_1 and s_2 with $s_1 > 2$ and $s_2 < -2$. This yields that there exists four roots $\{w_i\}_{i=1}^4$ of (5.5) that satisfy $w_1 > 1, w_2 < 1, -1 < w_3 < 0$ and $w_4 < -1$. Moreover, the roots satisfy

$$\begin{aligned} w + w^{-1} &= s_1, & w &= w_1, w_2, \\ w + w^{-1} &= s_2, & w &= w_3, w_4. \end{aligned}$$

To sum up, there exists four distinct roots for (5.4) such that two inside the unit disk while the other two outside the unit circle. To sum up, we require three boundary conditions, which is consistent with (5.2).

We next verify Assumption C for the coupling scheme.

For mode I, we have the following form of the solution

$$z(x_i, \theta) = c_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix} z_1^i + c_2 \begin{pmatrix} 0 \\ 1 \end{pmatrix} z_2^i + c_3 \begin{pmatrix} 0 \\ 1 \end{pmatrix} z_3^i, \quad |z_i| < 1, \quad i = 1, 2, 3.$$

where z_1 denotes the root of (5.3) with norm less than 1. z_2 and z_3 are the roots of (5.4) with norm less than 1. As $\theta \rightarrow 0$, we have $|z_1|, |z_2| \rightarrow 1$ while $|z_3| \rightarrow 3 - 2\sqrt{2}$. Substituting the above expression into the boundary condition, we obtain

$$\begin{pmatrix} 1 & -1 & -1 \\ z_1 & -z_2 & -z_3 \\ z_1^{-1} & -z_2^{-1} & -z_3^{-1} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}.$$

The determinant of the matrix is

$$\frac{(z_1 - z_2)(z_2 - z_3)(z_3 - z_1)}{z_1 z_2 z_3} \neq 0$$

because of the following lemma, whose proof is deferred to the end of this section.

Lemma 5.1. z_1, z_2 and z_3 are distinct roots.

We conclude that there does not exist mode I eigenfunction.

For mode II, notice that by definition,

$$(\bar{\mathcal{H}}_{\text{CB}}(\partial_x, \theta)w)(x) = 6(\partial_x^2 - \theta^2)w(x) = 0,$$

it is clear the only solution satisfying $w(x) \rightarrow 0$ as $x \rightarrow \pm\infty$ is the trivial solution $w(x) \equiv 0$, hence mode II eigenfunction does not exist.

For mode III, we have $\zeta \rightarrow 1$ as $\theta \rightarrow 0$. The solution takes the form

$$z = c \begin{pmatrix} 0 \\ 1 \end{pmatrix} z_3^i \quad \text{with} \quad z_3 = 2\sqrt{2} - 3,$$

substituting the above expression into the boundary condition, we obtain

$$c \begin{pmatrix} 0 \\ 1 \end{pmatrix} z_3^{-1} = c \begin{pmatrix} 0 \\ 1 \end{pmatrix} z_3,$$

which yields $c = 0$. This concludes that there does not exist mode III eigenfunction.

Therefore, the coupling scheme is stable and convergent.

Proof of Lemma 5.1. It is clear that

$$z_2 = w_2 \zeta^{1/2} \quad \text{and} \quad z_3 = w_3 \zeta^{1/2}$$

with $-1 < w_3 < 0 < w_2 < 1$, this implies $z_2 \neq z_3$.

A direct calculation gives

$$\begin{aligned} z_1 &= \frac{6 - \zeta - \bar{\zeta} - \sqrt{(4 - \zeta - \bar{\zeta})(2 - \zeta - \bar{\zeta})}}{2(1 + \bar{\zeta})} \\ &= \frac{6 - \zeta - \bar{\zeta} - \sqrt{(4 - \zeta - \bar{\zeta})(2 - \zeta - \bar{\zeta})}}{2(1 + \zeta)(1 + \bar{\zeta})} (1 + \zeta) \\ &= \frac{6 - \zeta - \bar{\zeta} - \sqrt{(4 - \zeta - \bar{\zeta})(2 - \zeta - \bar{\zeta})}}{2(2 + \zeta + \bar{\zeta})} (\zeta^{1/2} + \bar{\zeta}^{1/2}) \zeta^{1/2}. \end{aligned}$$

Recalling $\zeta = e^{i\theta}$ with $\theta \in (-\pi, \pi)$, and we may write

$$z_1 = \frac{2 \cos(\theta/2)}{3 - \cos \theta + \sqrt{(7 - \cos \theta)(1 - \cos \theta)}} e^{i\theta/2}.$$

Note that

$$\frac{2 \cos(\theta/2)}{3 - \cos \theta + \sqrt{(7 - \cos \theta)(1 - \cos \theta)}} > 0 > w_3,$$

this implies $z_1 \neq z_3$.

It remains to prove $z_1 \neq z_2$. Note that

$$z_2 = \frac{1}{2} (B - \sqrt{B^2 - 4}) e^{i\theta/2}$$

with

$$B = -A/2 + \sqrt{A^2/4 + 14 - (\zeta + \bar{\zeta})}.$$

Using

$$A = \zeta + \bar{\zeta} + \zeta^3 + \bar{\zeta}^3 = (\zeta + \bar{\zeta})(\zeta^2 + \bar{\zeta}^2) = 4 \cos(\theta/2) \cos \theta,$$

we write

$$\begin{aligned} A^2/4 + 14 - (\zeta + \bar{\zeta}) &= 16 \cos^2(\theta/2) \cos^2 \theta + 14 - 2 \cos \theta \\ &= 16 \cos^2(\theta/2) \cos^2 \theta + 14 - 2(2 \cos^2(\theta/2) - 1) \\ &= 16 - 4 \cos^2(\theta/2) \sin^2 \theta. \end{aligned}$$

This gives

$$B = 2\sqrt{4 - \cos^2(\theta/2) \sin^2 \theta} - 2 \cos(\theta/2) \cos \theta.$$

To prove $z_1 \neq z_2$, it remains to show $|z_1| \neq |z_2|$, i.e.,

$$\frac{1}{2} \left(B - \sqrt{B^2 - 4} \right) \neq \frac{2 \cos(\theta/2)}{3 - \cos \theta + \sqrt{(7 - \cos \theta)(1 - \cos \theta)}}.$$

Actually, we shall prove that for $\theta \in (-\pi, \pi)$ and $\theta \neq 0$, there holds

$$(5.6) \quad \frac{1}{2} \left(B - \sqrt{B^2 - 4} \right) > \frac{2 \cos(\theta/2)}{3 - \cos \theta + \sqrt{(7 - \cos \theta)(1 - \cos \theta)}}.$$

The above inequality is equivalent to

$$(5.7) \quad 3 - \cos \theta + \sqrt{(7 - \cos \theta)(1 - \cos \theta)} > \cos(\theta/2) \left(B + \sqrt{B^2 - 4} \right).$$

Denote by $t = \cos(\theta/2)$, we write the above inequality as

$$(5.8) \quad 2 - t^2 + \sqrt{(4 - t^2)(1 - t^2)} > t \left(g(t) + \sqrt{g^2(t) - 1} \right), \quad t \in [0, 1),$$

where

$$g(t) := t - 2t^3 + 2\sqrt{1 - t^4 + t^6}.$$

To prove (5.8), we firstly prove

$$(5.9) \quad 2 - t^2 > tg(t) \quad t \in [0, 1).$$

A direct calculation gives

$$\begin{aligned} 2 - t^2 - tg(t) &= 2(1 - t^2) + 2t \left(t^3 - \sqrt{1 - t^4 + t^6} \right) \\ &= 2(1 - t^2) + \frac{2t(t^4 - 1)}{\sqrt{1 - t^4 + t^6} + t^3} \\ &= 2(1 - t^2) \left(1 - \frac{t + t^3}{\sqrt{1 - t^4 + t^6} + t^3} \right). \end{aligned}$$

Note that

$$\sqrt{1 - t^4 + t^6} > t,$$

which follows from $(1 - t^2)(1 - t^4) > 0$. Combining the above two inequalities, we obtain (5.9).

Next, by (5.9) and note $g(t) \geq 0$, we obtain

$$(4 - t^2)(1 - t^2) = (2 - t^2)^2 - t^2 \geq t^2(g^2(t) - 1).$$

A direct calculation gives that $g(t) \geq 1$. Therefore,

$$\sqrt{(4 - t^2)(1 - t^2)} \geq t\sqrt{g^2(t) - 1},$$

which together with (5.9) gives (5.8). This implies $z_1 \neq z_2$ and completes the proof. \square

6. CONCLUSION

We have identified stability conditions, especially stability conditions at the interface, for atomistic-to-continuum hybrid methods with sharp interface. Under these stability conditions, we establish convergence of the hybrid scheme. While we only consider the flat interface here, the analysis can be extended to smooth interface between the atomistic and continuum regions. In that case, we need to check the interface stability condition Assumption C for interface with different angles.

For the example of atomistic-to-continuum coupling for triangular lattice considered here, the stability can be checked by hand. For many other more complicated interactions, this might not be easy or even possible to do by hand. One possible direction is to use numerical or symbolic computations to check stability conditions, in analogy to checking GKS conditions for example as in [32]. This is an interesting future research direction.

The result in this paper does not apply to transition interface between atomistic and continuum regions that involves corners. Extension of the result to hybrid schemes with transition interface with corners would be very interesting.

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